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Design novel 3D nano-architectures for developing ultra fast thermal energy storage materials

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14. ABSTRACT
In 2008 This team developed "pillared graphene" which was shown to have fast thermal energy transport. This grant used multi-scale modeling to design sp2 materials based on SiC and BN nanotubes, attempting to create junctions in such a way that all atoms will be of SP2 character (to optimize energy transfer). This examination of the junctions' structural and energetic characteristics allowed extension of the work to design of nanomaterials with ultrafast electron and phonon transport properties. The team assembled a variety of nanostructures for characterization, and moved on to pillared nanotube structures. The report itself is lightweight but the bulk of the detailed findings are in two published papers.

15. SUBJECT TERMS
EOARD, pillared graphene, graphene, energy transport, density functional theory, multiscale modeling

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FINAL TECHNICAL REPORT

Project Title : **Design novel 3D nano-architectures**

for developing ultra fast thermal energy storage materials

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Abstract:

In the 1st year of the grant we develop novel approaches to ultra fast thermal energy storage materials for Air Force Applications using novel 3D nano architectures. We applied a multi-scale computational approach to design novel sp2 nano-architectures based in SiC and BN Nanotubes. We used first principle ab-initio methods for studying the structural, bonding and energetic characteristics of the junctions and verify their stability.

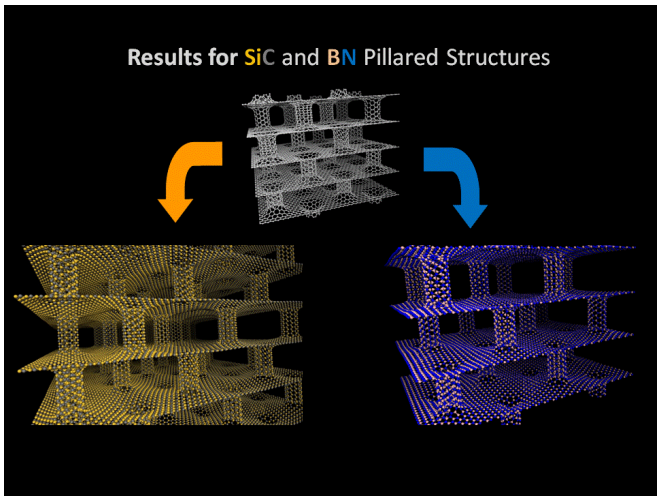
In the 2nd and 3rd year of the grant we design novel nano-materials with ultra fast electron and phonon transport properties for Air Force applications using 3D nano architectures based in SiC and BN. A variety of SiC and BN nanostructures with different geometrical characteristics were properly assembled. Then we designed different SiC & BN pillared models and their structural and electronic properties were investigated by multi-scale computational techniques.

1st FY Research

Project Title : Design novel 3D nano-architectures for developing ultra fast thermal energy storage materials

State of the art:

In 2008 we designed a C nano-architecture named Pillared Graphen [1-fig] that was proved later in 2010 to have ultra fast thermal energy transport [2]. This was attributed to the sp2 character of the C atoms, that do not scatter the phonons and to the tunable porosity of the structure.



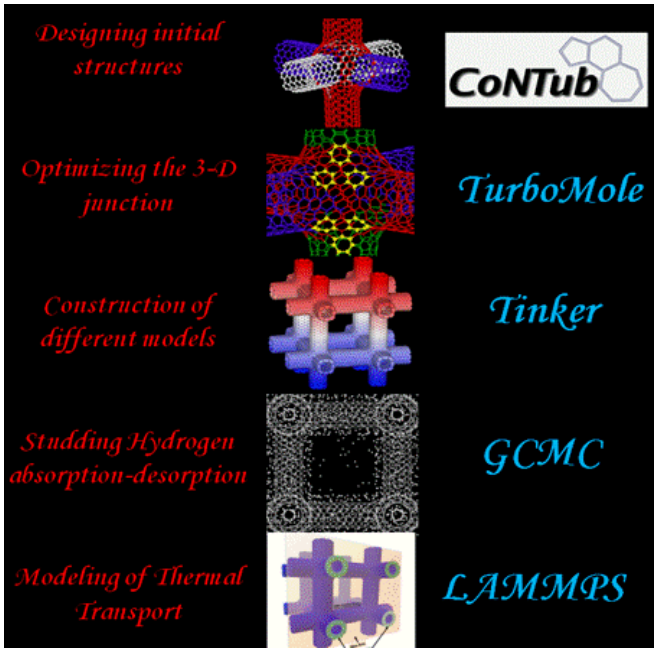
Objective:

Design novel sp2 nano-architectures based in SiC [3] and BN [4] Nanotubes.

Methodology:

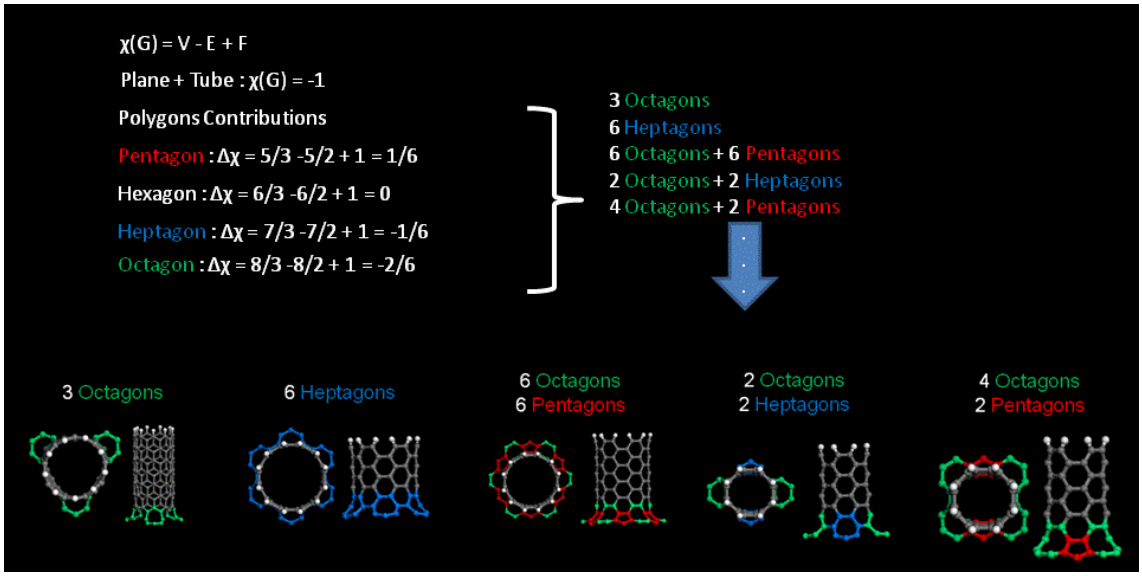
We applied a multi-scale computational approach as can be seen in the figure.

Both quantum chemical accurate calculations and Molecular Dynamics (MD) together with Monte Carlo (MC) simulations were involved. The work is physically divided in 5 different and complimentary tasks, schematically presented in figure.



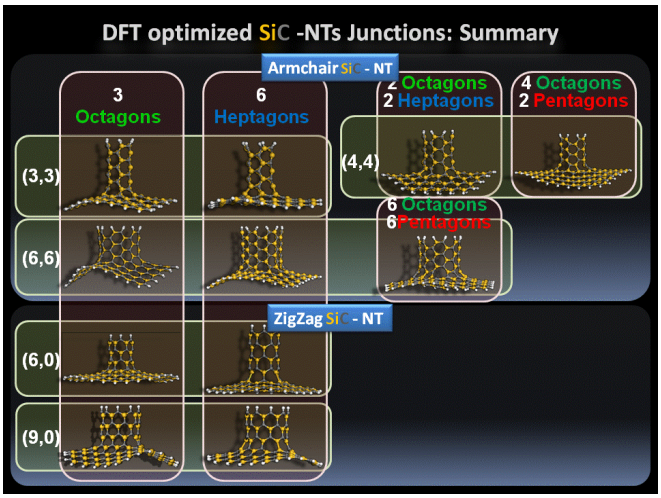
Designing initial structures : Euler's rules for connecting polygons

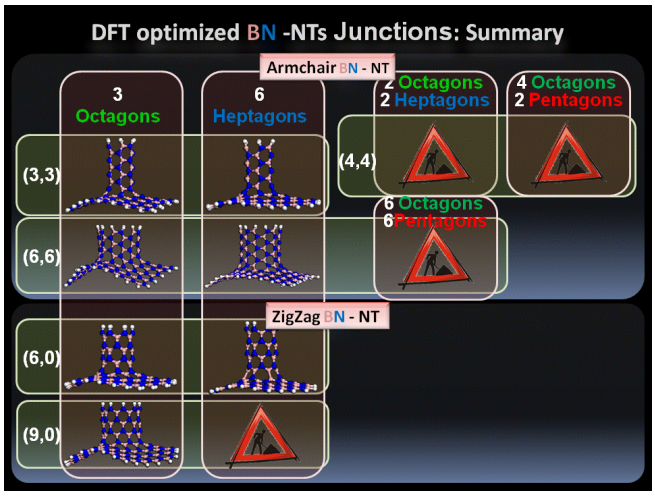
The key point is how to create a chemically stable junction in a way that all BN and SiC atoms will be of sp2 character. This was achieved by fallowing the Euler's rules for polygons (figure). For this purpose we used the CoNTube mathematical tool.



Checking the stability of the obtained 3D junction with DFT methods.

First principle ab-initio methods were used for studying the structural, bonding and energetic characteristics of the junctions and verify their stability. For this task we used Density Functional Theory (DFT) in the RI approximation as implemented in the TurboMole program package.





Publicity so far : <u>Invited talks</u>

- "Materials for hydrogen storage – future perspectives" on "Hurtigruten" (Norwegian Coastal Express) 14-18 June 2012. Title:" Designing Nanoporous Materials for Hydrogen Storage"
- NANOFUN Colloquium, Jacobs University, Bremen, Germany Jun 19 2012 Title:" Designing Nanoporous Materials for Hydrogen Storage"
- International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications, Athens 8-9 November 2012. Title:" Designing Nanoporous Materials for Hydrogen "

References

1. "Pillared Graphene: A New 3-D Network Nanostructure for Enhanced Hydrogen Storage", Dimitrakakis, G. K.; Tylianakis, E.; Froudakis, G. E. NanoLetters 8 (2008) 3166-3170.

2. "Modeling of Thermal Transport in Pillared-Graphene Architectures", V. Varshney, S. Patnaik, A. Roy, G.E. Froudakis, B. Farmer, ACS Nano 4 (2010) 1153–1161.

3. "SiC nanotubes: A novel material for hydrogen storage", Mpourmpakis G, Froudakis GE, et.al., Nano Letters 6 (2006) 1581.

4. "Why boron nitride nanotubes are preferable to carbon nanotubes for hydrogen storage? An ab initio theoretical study" G. Mpourmpakis, G. E. Froudakis, Catalysis Today, 120, 341 (2007).

2nd & 3rd FY Research

Project Title : Design novel 3D nano architectures based in SiC and BN with extraordinary electronic, magnetic and phonon transport properties

State of the art:

The ideal graphene [1] corresponds to a 100% sp^2 hybridised C-atoms but intensive study of nanocarbons has elucidated the role of the edges of graphene sheets and topological defects, such as vacancies, pentagons, heptagons producing curvature of the sp^2-clusters, which in nanoscale objects strongly influences their *electronic structure* and *magnetic properties* [2]. The insertion of "imperfections" is a way to modify the electronic and crystal structure of graphene, which is proved to be important for *graphene based nanoelectronics* [3].

Objective:

1. design 3D nano-architectures of SiC and BN and

2. study their electronic, magnetic and phonon transport properties.

Methodology:

We applied a multi-scale computational approach as can be seen in the figure 1.

Both quantum chemical accurate calculations and Molecular Dynamics (MD) together with Monte Carlo (MC) simulations were involved. The work is physically divided in 5 different and complimentary tasks, schematically presented in figure1.

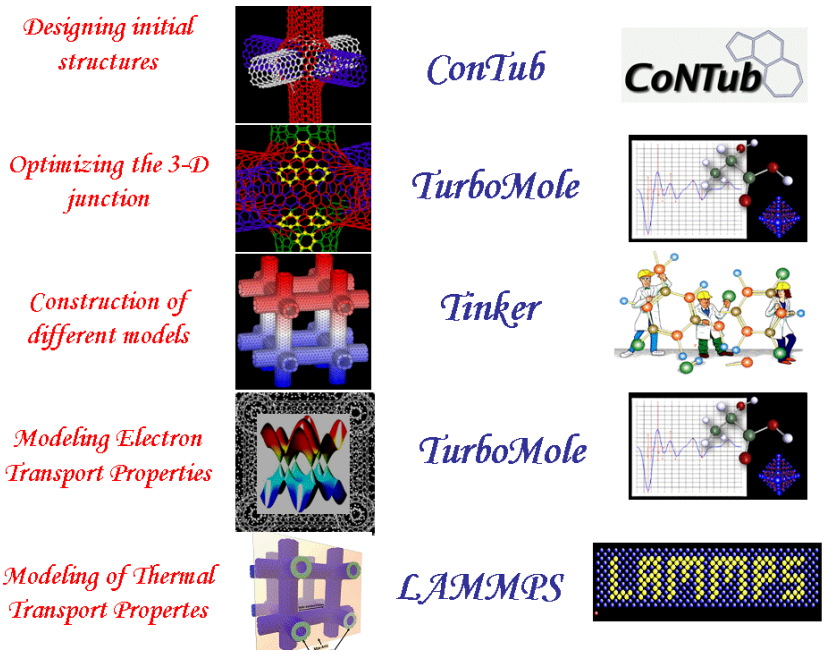


Figure 1: The 5 different tasks constructing the multi-scale methodology of the project together with the programs that will be used.

- Construction of the different SiC & BN pillared models.
  A variety of nanostructures with different geometrical characteristics were be properly assembled as can be seen in figure 2.

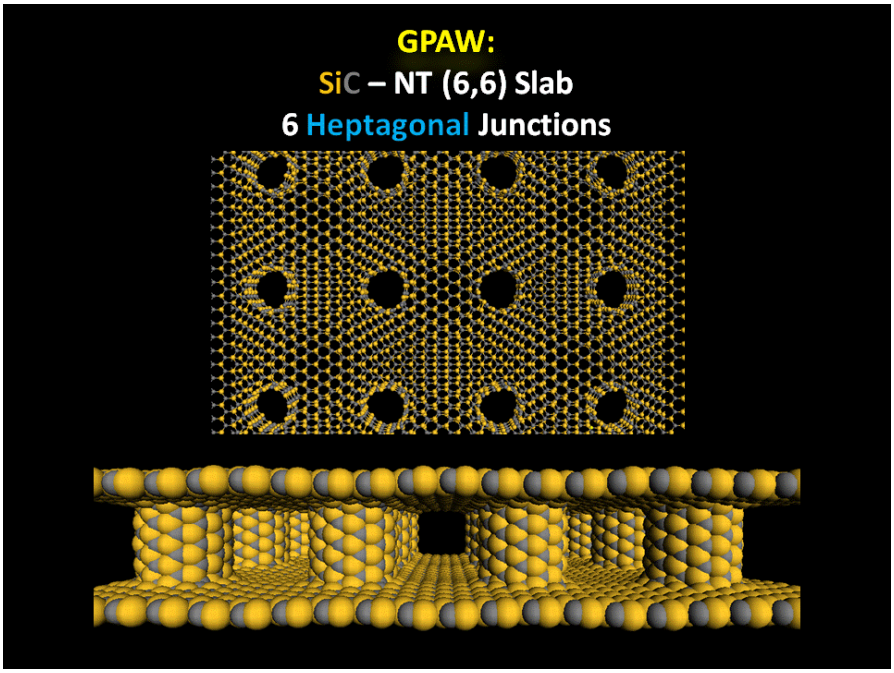


Figure 2: A periodic SiC-NT pillared structures optimized with the GPAW method

- Study of the electronic properties of SiC and BN pillared structures as can be seen in figure 3.

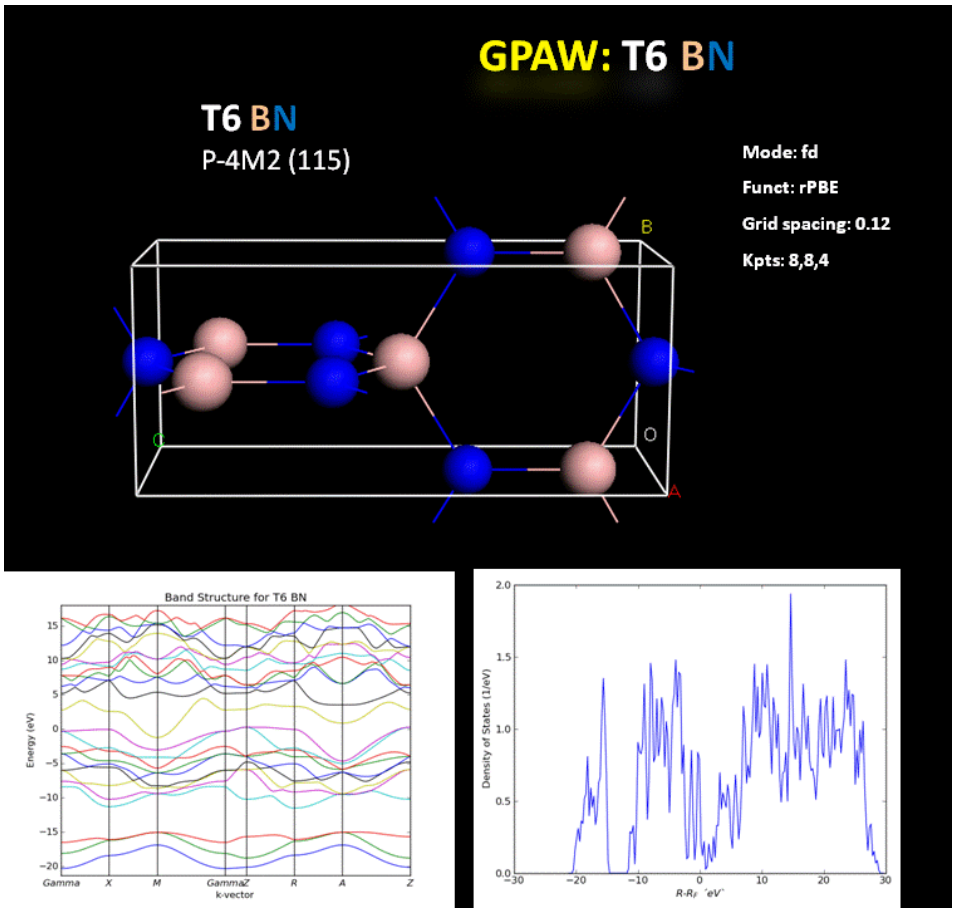


Figure 3: A periodic BN-NT pillared structure optimized with the GPAW method. The building unit, the band structure and the DOS.

Publicity so far : <u>Invited talks</u>

- "Materials for hydrogen storage – future perspectives" on "Hurtigruten" (Norwegian Coastal Express) 14-18 June 2012. Title:" Designing Nanoporous Materials for Hydrogen Storage"
- NANOFUN Colloquium, Jacobs University, Bremen, Germany Jun 19 2012 Title:" Designing Nanoporous Materials for Hydrogen Storage"
- International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications, Athens 8-9 November 2012. Title:" Designing Nanoporous Materials for Hydrogen "

Publicity so far : <u>Scientific publications</u>

1. "Separation of CO2-N-2 mixtures in 3D carbon-based porous nanotube networks: a molecular dynamics investigation`", I. Skarmoutsos, G. Tamiolakis, G. E. Froudakis, **PCCP Communication 16 (2014) 876-879**
2. "Designing Novel Nanoporous Architectures of Carbon Nanotubes for Hydrogen Storage", E. Tylianakis, G. Dimitrakakis, F. Martin-Martinez, S. Melchor, J.A. Dobado and G.E. Froudakis, submitted to **International Journal of Hydrogen Energy.**

References

1. "Pillared Graphene: A New 3-D Network Nanostructure for Enhanced Hydrogen Storage", Dimitrakakis, G. K.; Tylianakis, E.; Froudakis, G. E. NanoLetters 8 (2008) 3166-3170.

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